Stable corrugated state of the two-dimensional electron gas

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A corrugated and stable ground state is found for the two-dimensional electron gas in both the normal paramagnetic and the fully polarized phases. The self-consistent Hartree-Fock method is used with a modulated set of trial wave functions within the deformable jellium model. The results for high metallic densities reproduce the usual noncorrugated ferromagnetic electron-gas behavior. A transition to a paramagnetic corrugated state for values of $r_s \approx 6.5$ is predicted. At lower densities $r_s \approx 30$, a second transition to a corrugated ferromagnetic phase is suggested.

The electron gas is a cornerstone of the many-body quantum theory applications to solid-state physics [1]. Much effort has been devoted recently to the study of this system in the two-dimensional (2D) case. A wide range of important applications have led these studies. Among these one can mention the study of metal-oxide-semiconductor structures, heterostructures and superlattices [2], and the transport properties of semiconductors [3]. Also, in the presence of a magnetic field a two-dimensional system develops new interesting properties such as the fractional statistics and the quantum Hall effect [4,5]. Most notably, the electronic motion in the new high-temperature superconducting materials occurs mostly in planes [6,7].

In this work, the deformable jellium (DJ) within the unified framework provided by the Hartree-Fock method as done by Roothann [8] is applied to the 2D electron gas. Our aim is to evaluate the ground-state properties, especially the transition point to the corrugated state and to search for the existence of a (meta)stable state in the low-density region. In previous calculations a transition to a corrugated state in the 2D or 3D systems has been obtained; see, for example, Refs. [9–13]. However, the stability of the new corrugated state against density variations was not established before.

A recurrent problem in the study of the low-density transition to the Wigner crystal is the instability of the electron gas with respect to density variations. The usual way out of this problem is to postulate that the background compensates this instability. This solution is especially difficult to justify in the DJ model because the static part of the background energy is already incorporated into the model. One might always argue that some unknown dynamical effect could solve the problem, but this approach only postpones the conceptual difficulty. It would be logically much better if the electron system in the corrugated phase would exhibit a stable behavior. In the past, some indication of such a stable HF ground state has been reported by us for the 3D electron gas [14]. However, this was considered only a preliminary result because the convergence of the calculation was not good enough at low densities.

The standard *ab initio* studies of the electron gas assume a simplified model for the background. A usual assumption is the so-called (uniform) jellium model, in which the neutralizing positive background is taken to be a uniform static charge distribution [15]. Recently several techniques have been used to solve this model for the 2D case; these include the variational correlated-basis-function approach, the ladder approximation, and the effective-potential expansion method [16–18]. Perhaps the most ambitious calculations in the uniform jellium (UJ) are those that use the variational Monte Carlo and the Green's-function Monte Carlo (GFMC) methods [13]. However, these numerical solutions are in practice restricted to a few hundred particles [11,12].

A different hypothesis for the behavior of the background is the DJ [9,10]. Here the basic assumption is that the background is statically deformed in order to get local charge neutrality, simulating in this way some of its expected properties.

The DJ together with the much maligned Hartree-Fock (HF) method has been exploited by us in the study of the 3D electron gas. Our approach has been to obtain self-consistency with a set of modulating functions that contain as a possible solution the trivial plane wave [19].

This has turned in a very powerful technique that has the built-in capability of describing *both* the metallic and the low-density regions in a *unified* nonperturbative fashion. At metallic densities, $r_s \approx 4$, the plane-wave function is the self-consistently obtained ground state. Thus, in this region the DJ coincides with the UJ. At intermediate densities the corrugated solution has been obtained for the 3D electron gas [14]. At very low densities this solution approaches the Wigner crystal [20].

The deformable and the usual UJ models can be considered as two different extreme static behaviors of an actual background for which the charge density is neither locally neutral nor uniform. In both models the dynamical behavior of the background is as a first step neglected. The difference between the UJ and DJ amounts to a correlation [21] when the plane-wave solution is not the HF ground state of the DJ. In this sense, the DJ admits HF solutions that include a large correlation *with respect to* the HF solutions of the UJ. The origin of the correlation is perhaps more clearly seen if one abandons the static approximation for the background. In such a description the correlation arises from the electron-background interaction. Within this dynamic treatment the two models would differ by a class of (correlated) diagrams that includes those that relate the UJ and DJ background configurations. This difference is analogous to the one occurring with the spontaneous symmetry-breaking mechanism of field theory.

In general, the corrugated phase of the DJ predicts a lower ground state than the UJ. This result has again a close parallel with the spontaneous symmetry-breaking mechanism, where the "*true*" ground state is the less-symmetric one. One can also understand the improvement brought by the DJ in terms of a simple electrostatic analog, in which the condition of local neutrality is the most favorable energetically. Because, once in the corrugated region, the DJ model resembles the lattice localization, it could be a better starting point for more accurate calculations.

Consider the system of N electrons, interacting via a Coulomb potential $V(r_{ij})=e^2/r_{ij}$, where $r_{ij}=|r_i-r_j|$, immersed in a positive background in an area A. If the thermodynamic limit is considered, then $N\to\infty$, $A\to\infty$ with $\sigma=N/A$ constant. Schematically, the HF Hamiltonian equation of this system has the terms $H=T_e+V_{bb}+V_{be}+V_D+V_{\rm ex}$; where the subindices e and b refer to electron and background, respectively, and V_D and $V_{\rm ex}$ are the direct and exchange terms of the electron-electron interaction. V is the Coulomb interaction and T_e is the electronic kinetic energy. Atomic units are used throughout this work.

The condition that defines the DJ is [22] $\langle V_D\rangle+\langle V_{bb}\rangle+\langle V_{be}\rangle=0$, i.e., the terms of the background energy are identically canceled with the direct local term of the particle-particle interaction. The consequences of this hypothesis and the conditions under which it is satisfied have been discussed in a previous work [23].

The trial state functions in the Fock space are taken to be the usual PW's multiplied by modulating functions. The minimal modulating frequency q_0 is obtained via the orthonormality condition of the orbitals [19]. The proposed orbitals are of the form

$$\varphi_\kappa(\mathbf{r})=\frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{\sqrt{A}}\sum_{n_x,n_y=0}^{\mathcal{N}} C_{n_x n_y}\cos(q_0 n_x x)\cos(q_0 n_y y)\ , \tag{1}$$

where A is the area in which the periodic boundary conditions are imposed. The coefficients C_{n_x,n_y} are assumed to be independent of k. These coefficients are self-consistently determined by the HF equations with the orthonormality condition included. The first term in this expansion $n_x=n_y=0$ is the PW solution. For the upper limits in the sums we select $\mathcal{N}_x=\mathcal{N}_y=\mathcal{N}$; in that way, when the solution is different from the PW, the system has a periodic density centered on a square lattice. The number of terms for this lattice increases like $(\mathcal{N}+1)^2$. Other lattices can be obtained by the usual modification of the Brillouin-zone geometry. Although in the 2D system one expects that the hexagonal lattice will be the most favorable energetically, we will show that even for the square lattice the DJ gives a better energy than any UJ calculation performed so far.

The energies for the normal paramagnetic state and for the fully polarized one are evaluated in order to determine the magnetic nature of the ground state. In the paramagnetic case, each orbital within the Fermi sphere of radius k_F has double occupancy, while in the ferromagnetic case the orbitals within a sphere of radius $\sqrt{2}k_F$ are singly occupied. The ground-state energy per particle with the orbitals of Eq. (1) requires the evaluation of terms of the form

$$\frac{T}{N}=\frac{1}{r_s^2}\sum_{\mathbf{n}}|C_{\mathbf{n}}|^2(1+8\mathbf{n}^2) \tag{2}$$

for the expectation value of the one-particle kinetic energy, and

$$\frac{V}{N}=-\frac{\sqrt{2}/(32\pi^2)}{r_s}\sum_{\mathbf{n}_1}\sum_{\mathbf{n}_2}\sum_{\mathbf{n}_3}\sum_{\mathbf{n}_4} C^*_{\mathbf{n}_1}C^*_{\mathbf{n}_2}C_{\mathbf{n}_3}C_{\mathbf{n}_4}I(\mathbf{n}_1,\mathbf{n}_4)\times F(\mathbf{n}_1,\mathbf{n}_2,\mathbf{n}_3,\mathbf{n}_4) \tag{3}$$

for the nonlocal exchange term of the two-body Coulomb potential. In these equations r_s is the density parameter in Bohr radius and N is the number of particles. $\mathbf{n}$ is a two-dimensional vector $\mathbf{n}=n_x\mathbf{i}+n_y\mathbf{j}$. The function $I(\mathbf{n}_1,\mathbf{n}_4)$ that stems from the integrals of the Coulomb potential has been numerically evaluated. Notice that the function $I(\mathbf{n}_1,\mathbf{n}_4)$ depends on two indices as it should be for the exchange part of a two-particle operator. Finally $F(\mathbf{n}_1,\mathbf{n}_2,\mathbf{n}_3,\mathbf{n}_4)$ is a sum of 64 terms that are products of Kronecker δ functions in the components of the four n_i's. The coefficients $C_{\mathbf{n}}$ were self-consistently determined with an approximation of 10^{-5} with respect to the previous iteration. The value of the upper limit in the sums was changed from $\mathcal{N}=1$ up to 16, in order to obtain results for the ground-state energy independent of $\mathcal{N}$. We get convergence for the energy results in a wide interval of $3<r_s<50$, with a function up to 289 terms. The evaluation of the ground-state energy for ten points with the $\mathcal{N}=16$ expansion required about 350 VAX-780

equivalent hours.

The difference in the ground-state energy per particle between the PW case and the self-consistent solution, in terms of the density parameter, is shown in Fig. 1. Convergence for the r_s value of the transition from the PW to the corrugated state is obtained for $\mathcal{N} \geq 3$. Notice that the transition appears at a greater density in the paramagnetic ($r_s = 4.8$) than in the ferromagnetic system ($r_s = 6.8$). The value obtained for the transition point in the 2D paramagnetic system is much lower than the result previously obtained in the corresponding 3D electron gas [14] of $r_s = 26$. This could be expected from the density-functional calculations of Ref. [24] and the GFMC method [13]. However, our transition values are significantly lower than the value of $r_s \approx 40$ obtained for the UJ model [13].

In Fig. 2, the ground-state energy per particle is plotted for the two phases. Immediately after the transition to periodic electronic density, the energy curves for $\mathcal{N} \geq 4$ show a region in which the slope changes. Then the curves with $\mathcal{N} = 16$ show a minimum at $r_s = 25$ in the normal system and at $r_s = 38$ for the fully polarized case. The slow convergence of the method does not allow us to distinguish between the presence of a minimum or of a shoulder for the actual curve of the HF-DJ system. In any case, there is a region of positive pressure that is followed at lower densities by either a point of stability or a region with a very small or null pressure. The scenario with a finite r_s minimum would be equivalent to the situation in the metallic density region (where the HF solution is the PW) and that supports the confidence in the electron-gas model for the metals [15]. A remarkable feature of our calculation is the possible existence of these new stable states. In Fig. 2, the results reported with the GFMC [13] for the 2D UJ are included. One can observe that, at intermediate and low densities $r_s \geq 10$, the 2D DJ has a lower energy than the UJ. No sign of minimum value for the energy as a function of r_s at these densities has been reported for the UJ calculations.

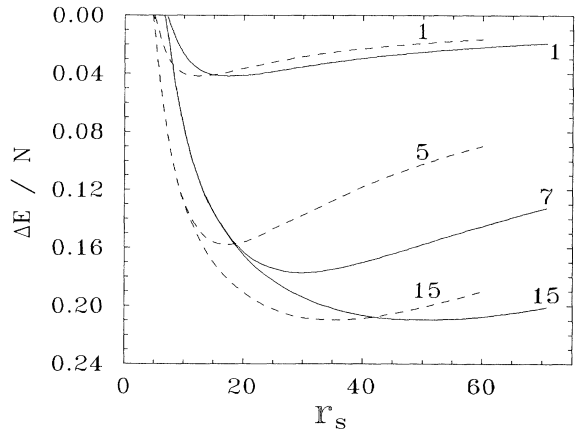

FIG. 1. Energy difference per particle, in rydbergs, between the trivial PW and the HF expansion of Eq. (1), as a function of the parameter r_s, in Bohr radius. The results are given for different values of $\mathcal{N}$. The various curves are labeled by the corresponding $\mathcal{N}$ value. Two sets of curves are given: dashed lines correspond to the paramagnetic system, while solid lines correspond to the ferromagnetic system.

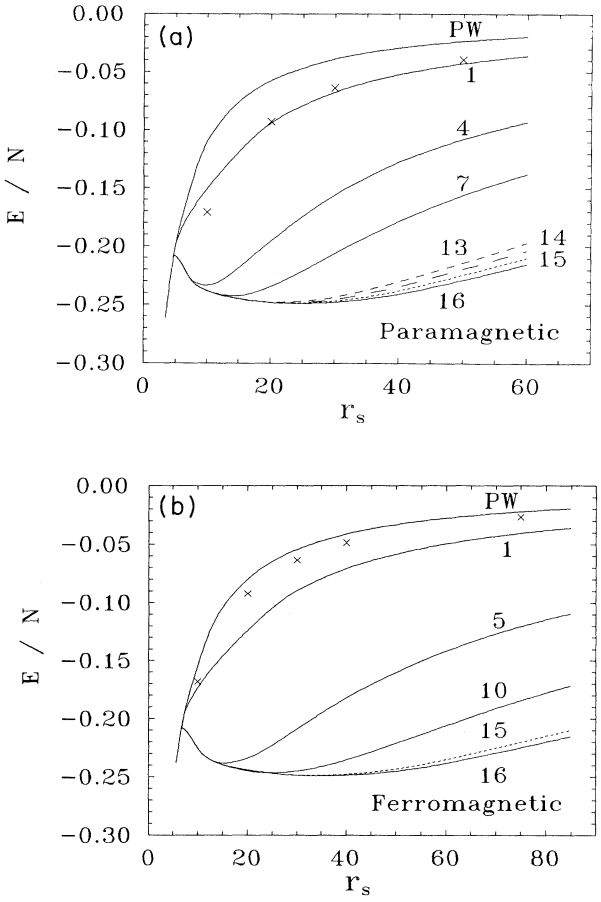

FIG. 2. Energy per particle, in rydbergs, as a function of r_s: (a) the paramagnetic system and (b) the ferromagnetic system. The different curves are labeled by the value of the corresponding $\mathcal{N}$. The crosses are the values given in Ref. [13].

It follows from Fig. 2(a) and Table I that satisfactory convergence in the energy is obtained in the intermediate

TABLE I. Ground-state energy per particle of the paramagnetic system as a function of the number of terms in the state function. The results are given at four different densities that involve the intermediate- and high-density region.

$\mathcal{N}$	$r_s = 10$	$r_s = 20$	$r_s = 30$	$r_s = 40$
0	−0.1100	−0.0575	−0.0389	−0.0294
1	−0.1503	−0.0941	−0.0674	−0.0524
3	−0.2222	−0.1706	−0.1312	−0.1057
5	−0.2376	−0.2137	−0.1764	−0.1474
7	−0.2381	−0.2345	−0.2063	−0.1786
9	−0.2381	−0.2436	−0.2256	−0.2019
11	−0.2381	−0.2469	−0.2371	−0.2186
13	−0.2382	−0.2478	−0.2436	−0.2303
15	−0.2382	−0.2481	−0.2469	−0.2381
16	−0.2382	−0.2481	−0.2479	−0.2409

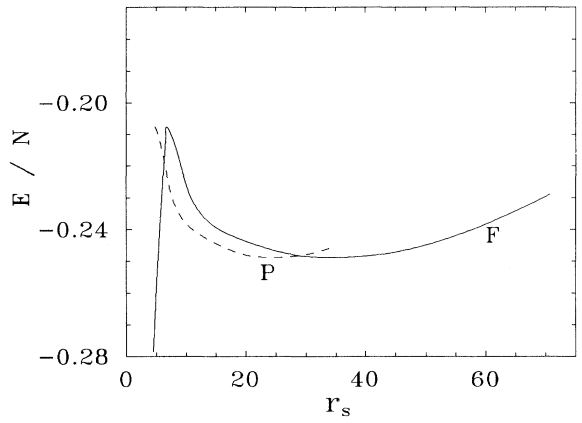

FIG. 3. Ground-state energy per particle, in rydbergs, of the 2D electron gas in terms of the parameter r_s. The solid line corresponds to the ferromagnetic phase and the dashed line to the paramagnetic one.

density region up to $r_s \approx 28$ for the paramagnetic phase. Figure 2(b) shows that a good convergence is obtained at densities up to $r_s \approx 50$ for the ferromagnetic energy. One would have to go to greater values of $\mathcal{N}$ if more accuracy in the energy were required at lower densities.

In conclusion, the DJ model confirms that the usual uniform PW solution in a ferromagnetic configuration is the HF ground state of the 2D electron gas with densities from $r_s \approx 2$ up to $r_s \approx 6.5$. At this point the system is predicted to have a transition to paramagnetic corrugated state; see Fig. 3 In this phase towards lower densities a positive pressure region is obtained. At $r_s \approx 30$, the fixed $\mathcal{N}=16$ curves of the electron gas show a magnetic transition to a ferromagnetic corrugated configuration. If a more precise calculation maintains this behavior, two metastable states would exist in this model, one paramagnetic at $r_s \approx 25$ and the second at $r_s \approx 38$, in the ferromagnetic configuration.

Just as the existence of the usual uniform HF state at metallic densities gives a good starting point for the many-body techniques that have been applied to the electron-gas system [15], the presence of these new stable states could be of great relevance, both from a conceptual and from a practical point of view. In principle, they provide a firm starting point from which more sophisticated calculations could be performed.

An important question not addressed in this work is what would be the effect of the non-spin-electron correlations on the ground state of the DJ. A partial answer can be obtained at least for static correlations by introducing a screened Coulomb interaction. In the past we have computed the effect of this type of interaction on the energy spectrum and on the ground-state energy of the 3D electron gas [19,25]. The only effect that one expects from this type of correlation is to move the transition point of the corrugated state to a lower density and, as the range of the interaction is diminished, to move the energy of the system up. Therefore the qualitative behavior of the possible metastable states would not be expected to change. The quantitative differences will depend on the strength of the screening, which could be expected to be small.

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